Piotr Cieplak

List of Publications by Year in descending order

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70 papers	29,918 citations	136885 32 h-index	102432 66 g-index
71 all docs	71 docs citations	71 times ranked	24748 citing authors

#	Article	IF	Citations
1	A Second Generation Force Field for the Simulation of Proteins, Nucleic Acids, and Organic Molecules. Journal of the American Chemical Society, 1995, 117, 5179-5197.	6.6	12,116
2	A well-behaved electrostatic potential based method using charge restraints for deriving atomic charges: the RESP model. The Journal of Physical Chemistry, 1993, 97, 10269-10280.	2.9	6,453
3	Calculating Structures and Free Energies of Complex Molecules:â€‰Combining Molecular Mechanics and Continuum Models. Accounts of Chemical Research, 2000, 33, 889-897.	7.6	4,098
4	Continuum Solvent Studies of the Stability of DNA, RNA, and Phosphoramidateâ^'DNA Helices. Journal of the American Chemical Society, 1998, 120, 9401-9409.	6.6	1,442
5	Application of RESP charges to calculate conformational energies, hydrogen bond energies, and free energies of solvation. Journal of the American Chemical Society, 1993, 115, 9620-9631.	6.6	1,229
6	Application of the multimolecule and multiconformational RESP methodology to biopolymers: Charge derivation for DNA, RNA, and proteins. Journal of Computational Chemistry, 1995, 16, 1357-1377.	1.5	944
7	A Modified Version of the Cornellet al.Force Field with Improved Sugar Pucker Phases and Helical Repeat. Journal of Biomolecular Structure and Dynamics, 1999, 16, 845-862.	2.0	882
8	Molecular mechanical models for organic and biological systems going beyond the atom centered two body additive approximation: aqueous solution free energies of methanol and N-methyl acetamide, nucleic acid base, and amide hydrogen bonding and chloroform/water partition coefficients of the nucleic acid bases. Journal of Computational Chemistry, 2001, 22, 1048-1057.	1.5	378
9	Polarization effects in molecular mechanical force fields. Journal of Physics Condensed Matter, 2009, 21, 333102.	0.7	236
10	Strike a balance: Optimization of backbone torsion parameters of AMBER polarizable force field for simulations of proteins and peptides. Journal of Computational Chemistry, 2006, 27, 781-790.	1.5	159
11	Epitope-resolved profiling of the SARS-CoV-2 antibody response identifies cross-reactivity with endemic human coronaviruses. Cell Reports Medicine, 2021, 2, 100189.	3.3	149
12	Development of Polarizable Models for Molecular Mechanical Calculations I: Parameterization of Atomic Polarizability. Journal of Physical Chemistry B, 2011, 115, 3091-3099.	1.2	137
13	Development of Polarizable Models for Molecular Mechanical Calculations II: Induced Dipole Models Significantly Improve Accuracy of Intermolecular Interaction Energies. Journal of Physical Chemistry B, 2011, 115, 3100-3111.	1.2	116
14	On the use of electrostatic potential derived charges in molecular mechanics force fields. The relative solvation free energy ofcis- andtrans-N-methyl-acetamide. Journal of Computational Chemistry, 1991, 12, 1232-1236.	1.5	107
15	Calculation of free energy changes in ionâ€“water clusters using nonadditive potentials and the Monte Carlo method. Journal of Chemical Physics, 1987, 86, 6393-6403.	1.2	81
16	The Wnt/Planar Cell Polarity Protein-tyrosine Kinase-7 (PTK7) Is a Highly Efficient Proteolytic Target of Membrane Type-1 Matrix Metalloproteinase. Journal of Biological Chemistry, 2010, 285, 35740-35749.	1.6	77
17	Molecular Dynamics Simulations Find That 3â€˜ Phosphoramidate Modified DNA Duplexes Undergo a B to A Transition and Normal DNA Duplexes an A to B Transition. Journal of the American Chemical Society, 1997, 119, 6722-6730.	6.6	76
18	Matrix Metalloproteinase Proteolysis of the Myelin Basic Protein Isoforms Is a Source of Immunogenic Peptides in Autoimmune Multiple Sclerosis. PLoS ONE, 2009, 4, e4952.	1.1	76

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19	Basis for substrate recognition and distinction by matrix metalloproteinases. Proceedings of the National Academy of Sciences of the United States of America, 2014, 111, E4148-55.	3.3	75
20	Structural Determinants of Limited Proteolysis. Journal of Proteome Research, 2011, 10, 3642-3651.	1.8	68
21	Monte Carlo simulation of aqueous solutions of Li+ and Na+ using manyâ€body potentials. â€‰Coordination numbers, ion solvation enthalpies, and the relative free energy of solvation. Journal of Chemical Physics, 1990, 92, 6761-6767.	1.2	67
22	Development of Polarizable Models for Molecular Mechanical Calculations. 4. van der Waals Parametrization. Journal of Physical Chemistry B, 2012, 116, 7088-7101.	1.2	60
23	Caspase Cleavage Sites in the Human Proteome: CaspDB, a Database of Predicted Substrates. PLoS ONE, 2014, 9, e110539.	1.1	59
24	S-Nitrosylation-Mediated Redox Transcriptional Switch Modulates Neurogenesis and Neuronal Cell Death. Cell Reports, 2014, 8, 217-228.	2.9	58
25	Free energy calculation on base specificity of drug - DNA interactions: Application to daunomycin and acridine intercalation into DNA. Biopolymers, 1990, 29, 717-727.	1.2	53
26	Development of Polarizable Models for Molecular Mechanical Calculations. 3. Polarizable Water Models Conforming to Thole Polarization Screening Schemes. Journal of Physical Chemistry B, 2012, 116, 7999-8008.	1.2	49
27	The Antimalarial Natural Product Salinipostin A Identifies Essential Î±/Î² Serine Hydrolases Involved in Lipid Metabolism in P.Âfalciparum Parasites. Cell Chemical Biology, 2020, 27, 143-157.e5.	2.5	48
28	Inflammatory Proprotein Convertase-Matrix Metalloproteinase Proteolytic Pathway in Antigen-presenting Cells as a Step to Autoimmune Multiple Sclerosis. Journal of Biological Chemistry, 2009, 284, 30615-30626.	1.6	39
29	Matrix metalloproteinases â€“ From the cleavage data to the prediction tools and beyond. Biochimica Et Biophysica Acta - Molecular Cell Research, 2017, 1864, 1952-1963.	1.9	39
30	A molecular mechanical model that reproduces the relative energies for chair and twist-boat conformations of 1,3-dioxanes. Journal of Computational Chemistry, 1995, 16, 243-261.	1.5	37
31	Selective function-blocking monoclonal human antibody highlights the important role of membrane type-1 matrix metalloproteinase (MT1-MMP) in metastasis. Oncotarget, 2017, 8, 2781-2799.	0.8	35
32	Resolving the Ligand-Binding Specificity in c-MYC G-Quadruplex DNA: Absolute Binding Free Energy Calculations and SPR Experiment. Journal of Physical Chemistry B, 2017, 121, 10484-10497.	1.2	34
33	CleavPredict: A Platform for Reasoning about Matrix Metalloproteinases Proteolytic Events. PLoS ONE, 2015, 10, e0127877.	1.1	32
34	S-nitrosylated TDP-43 triggers aggregation, cell-to-cell spread, and neurotoxicity in hiPSCs and in vivo models of ALS/FTD. Proceedings of the National Academy of Sciences of the United States of America, 2021, 118, .	3.3	28
35	High-Throughput Multiplexed Peptide-Centric Profiling Illustrates Both Substrate Cleavage Redundancy and Specificity in the MMP Family. Chemistry and Biology, 2015, 22, 1122-1133.	6.2	26
36	Development of Polarizable Gaussian Model for Molecular Mechanical Calculations I: Atomic Polarizability Parameterization To Reproduce ab Initio Anisotropy. Journal of Chemical Theory and Computation, 2019, 15, 1146-1158.	2.3	26

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37	High Throughput Substrate Phage Display for Protease Profiling. Methods in Molecular Biology, 2009, 539, 93-114.	0.4	23
38	S-Nitrosylation of p62 Inhibits Autophagic Flux to Promote Î±-Synuclein Secretion and Spread in Parkinson's Disease and Lewy Body Dementia. Journal of Neuroscience, 2022, 42, 3011-3024.	1.7	22
39	Walking on the free energy hypersurface of the 18â€crownâ€6 ion system using free energy derivatives. Journal of Chemical Physics, 1994, 101, 627-633.	1.2	20
40	Sequenceâ€derived structural features driving proteolytic processing. Proteomics, 2014, 14, 42-50.	1.3	20
41	Efficient formulation of polarizable Gaussian multipole electrostatics for biomolecular simulations. Journal of Chemical Physics, 2020, 153, 114116.	1.2	19
42	Elucidating the Origin of Conformational Energy Differences in Substituted 1,3-Dioxanes:Â A Combined Theoretical and Experimental Study. Journal of Organic Chemistry, 1996, 61, 3662-3668.	1.7	17
43	Penultimate unit effects in the free-radical copolymerization of styrene with acrylonitrile according to theoretical thermochemistry. Journal of Polymer Science Part A, 2002, 40, 3592-3603.	2.5	16
44	Conformations of Duplex Structures Formed by Oligodeoxynucleotides Covalently Linked to the Intercalator 2-Methoxy-6-Chloro-9-Aminoacridine. Journal of Biomolecular Structure and Dynamics, 1987, 5, 361-382.	2.0	12
45	Effect of phosphorylation and single nucleotide polymorphisms on caspase substrates processing. Apoptosis: an International Journal on Programmed Cell Death, 2018, 23, 194-200.	2.2	12
46	PyRESP: A Program for Electrostatic Parameterizations of Additive and Induced Dipole Polarizable Force Fields. Journal of Chemical Theory and Computation, 2022, 18, 3654-3670.	2.3	12
47	Application of the quantum mechanics and free energy perturbation methods to study molecular processes. International Journal of Quantum Chemistry, 1987, 32, 65-74.	1.0	11
48	Reply to: â€˜â€˜Comment on â€˜Waterâ€“water and waterâ€“ion potential functions including terms for manyâ€body effects,â€™ T. P. Lybrand and P. Kollman, J. Chem. Phys. 83, 2923 (1985) and on â€˜Calculation of free energy changes in ionâ€“water clusters using nonadditive potential and the Monte Carlo methods,â€™ P. Cieplak, T. P. Lybrand, and P. Kollman, J. Chem. Phys. 86, 6393 (1987)â€™â€™. Journal of Chemical Physics, 1988, 88, 8017-8017.	1.2	11
49	Matrix Metalloproteinase (MMP) Proteolysis of the Extracellular Loop of Voltage-gated Sodium Channels and Potential Alterations in Pain Signaling. Journal of Biological Chemistry, 2015, 290, 22939-22944.	1.6	11
50	Role of N-glycosylation in activation of proMMP-9. A molecular dynamics simulations study. PLoS ONE, 2018, 13, e0191157.	1.1	11
51	Induced polarization restricts the conformational distribution of a light-harvesting molecular triad in the ground state. Physical Chemistry Chemical Physics, 2017, 19, 22969-22980.	1.3	10
52	Stress tensor and constant pressure simulation for polarizable Gaussian multipole model. Journal of Chemical Physics, 2022, 156, 114114.	1.2	10
53	AmberFFC, a flexible program to convert AMBER and GLYCAM force fields for use with commercial molecular modeling packages. Journal of Molecular Modeling, 2001, 7, 422-432.	0.8	9
54	Novel procedure for thermal equilibration in molecular dynamics simulation. Molecular Simulation, 2009, 35, 349-357.	0.9	9

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55	A technique to study molecular recognition in drug design: Preliminary application of free energy derivatives to inhibition of a malarial cysteine protease. , 1996, 9, 103-112.		8
56	Molecular Design of Fluorine-Containing Peptide Mimetics. ACS Symposium Series, 1996, , 143-156.	0.5	7
57	Determining the atomic charge of calcium ion requires the information of its coordination geometry in an EF-hand motif. Journal of Chemical Physics, 2021, 154, 124104.	1.2	6
58	Amino acid sequence conservation of the algesic fragment of myelin basic protein is required for its interaction with CDK 5 and function in pain. FEBS Journal, 2018, 285, 3485-3502.	2.2	5
59	Quantitative profiling of protease specificity. PLoS Computational Biology, 2021, 17, e1008101.	1.5	5
60	CaspNeuroD: a knowledgebase of predicted caspase cleavage sites in human proteins related to neurodegenerative diseases. Database: the Journal of Biological Databases and Curation, 2016, 2016, baw142.	1.4	5
61	Toxoplasma gondii serine hydrolases regulate parasite lipid mobilization during growth and replication within the host. Cell Chemical Biology, 2021, 28, 1501-1513.e5.	2.5	4
62	Hydration of Benzoic Acid in Benzene Solution. Zeitschrift Fur Physikalische Chemie, 1992, 177, 63-74.	1.4	3
63	Letter to the Editor: Caspase cleavage sites in the human proteome: CaspDB, a database of predicted substrates. Apoptosis: an International Journal on Programmed Cell Death, 2015, 20, 421-421.	2.2	3
64	Interaction of the cryptic fragment of myelin basic protein with mitochondrial voltage-dependent anion-selective channel-1 affects cell energy metabolism. Biochemical Journal, 2018, 475, 2355-2376.	1.7	3
65	A Note on the Potential BCG Vaccination â€“ COVID-19 Molecular Link. Coronaviruses, 2020, 1, 4-6.	0.2	3
66	Application of the Free Energy Calculations to Study Drug-enzyme and Drug-dna Complexes. Molecular Simulation, 2002, 28, 173-186.	0.9	2
67	Peptide Sequence Region That is Essential for the Interactions of the Enterotoxigenic Bacteroides fragilis Metalloproteinase II with E-cadherin. Journal of Proteolysis, 2014, 1, 3-14.	0.0	2
68	Neglected N-Truncated Amyloid-Î² Peptide and Its Mixed Cuâ€“Zn Complexes. Protein Journal, 0, , .	0.7	1
69	Interactions between motor domains in kinesin-14 Ncd â€” a molecular dynamics study. Biochemical Journal, 2019, 476, 2449-2462.	1.7	0
70	Identifying protease cleavage sites by labelâ€free mass spectrometry. FASEB Journal, 2010, 24, 905.4.	0.2	0